COMMONWEALTH OF PENNSYLVANIA
DEPARTMENT OF ENVIRONMENTAL PROTECTION
BUREAU OF ENVIRONMENTAL CLEANUP AND BROWNFIELDS

UNSATURATED ZONE POTENTIAL MIGRATION MODEL

Spreadsheet name: BUFFER1.XLS

General Description: The primary purpose of this model is to estimate the movement of organic and inorganic species vertically through unsaturated zone soils toward bedrock/groundwater. This spreadsheet has been used to estimate the soil buffer distances in Tables 3B and 4B in Appendix A of the Act 2 regulations. The spreadsheet described here does not require a detailed knowledge of the specific compounds existing in the soil or soil properties. In addition, this spreadsheet is comparatively simple to use.

This spreadsheet relies on a relatively simple, straightforward methodology which allows the user to at least discern a trend of potential migration of inorganic or organic species vertically through the soil at a site. This is accomplished by first estimating an apparent partition coefficient by mathematically comparing total and leachate data for soils on-site. With this apparent partition coefficient and other input values, the spreadsheet can then make estimates of potential migration of the species through the unsaturated zone. Values for apparent partition coefficients for some inorganics can also be found in Appendix A Table 5B (as K_d values) or in the scientific literature.

For organics, apparent partition coefficients can be determined site- specifically or can be estimated as the product of the fraction organic carbon in soil and the K_{oc}. Values for K_{oc} can be found in Table 5A of the Act 2 regulations or in the scientific literature. See Section III.A.1. of the January 2019 Technical Guidance Manual for more detailed discussion of input values for unsaturated zone contaminant migration models.

The migration component of this model is based on contaminant depletion (mass balance) as infiltrating water moves through the contaminated soil and underlying uncontaminated soil. While this method of estimating migration of organic and inorganic species may seem somewhat oversimplified, it offers the user an easy-to-use option to other more complicated models (such as metal speciation models which currently exist). In addition, if the results of modeling potential migration of organics or inorganics with this spreadsheet indicate that a significant potential exists for groundwater to be degraded, a more rigorous modeling approach (such as a metal speciation model for metals) may be in order.

Application: This spreadsheet enables the user to estimate vertical migration of inorganic and organic species from contaminated soil to underlying soil through time. As such, its most useful application would probably be in determining whether or not a contaminant in soil may potentially reach groundwater, and to a lesser extent, what the concentration will be in soil pore water at the groundwater/vadose zone interface (if it does migrate to groundwater), and how long it will take for the contaminant to get there.

This spreadsheet could also be a useful component in making "what if" determinations with respect to remediation options. For example, if the uppermost 5 feet of soil is contaminated at a site, this spreadsheet could aid in determining what potential effect removal of a 1-foot or 2-foot depth of soil would have on subsequent vertical migration of the contaminant.

Required input: The major portion of this spreadsheet is output. The input ranges are B6 to B10 and C18 to C67. Following is a brief description of the needed input.

Cell B6 = recharge rate for the unsaturated zone soil in cm/yr. [As a cautionary note, if this value becomes unrealistically high (> 100 cm/yr), the output becomes very erratic. This is due to the computational formulas in the spreadsheet. These formulas could be modified with logic statements to prevent this problem; however, this would require much more memory resulting in a much more limited capability in terms of the number of time increments which could be modeled.]

Cell B7 = soil bulk density in g/cc. cell B8 = water-filled porosity of soil.

Cell B9 = apparent partition coefficient for inorganic or organic species in ml/g.

Cell B10 = depth increment in feet or thickness of soil layers being considered in feet. This is determined essentially from the contaminant concentrations in soil at varying depths obtained from on-site sampling. A value of one foot has been used in determining the buffer distances in Tables 3B and 4B of the Act 2 regulations.

Cells C18 to C67 = contaminant concentration in soil in mg/kg dry weight at each soil depth.

The input cells and ranges of cells in this spreadsheet are unprotected. The remaining cells of the spreadsheet are protected and are either labels (text), estimated values (from user input), or blank cells. It should be noted that disabling the protection of protected cells which contain mathematical formulas and making any changes could result in the loss of those formulas and could therefore destroy the capabilities of the spreadsheet. To avoid this, formulas in protected cells should not be changed.

Spreadsheet assumptions and equations: The following assumptions apply to this spreadsheet:

1. Homogeneous and isotropic conditions exist in the unsaturated zone soils.

2. Flow of water infiltrating vertically through the unsaturated zone is uniform.

3. Contaminant movement is only in the vertical direction - not lateral.

4. Contaminant concentrations are not so high as to affect the flow of water in the unsaturated zone.

5. Multiple contaminants act independently of each other.

6. For any species in soil, the relationship between the concentration "sorbed" and the aqueous concentration remains linear irrespective of concentration.

The equations upon which this model is based are actually located in the range of D18 to IT156 and are ordered according to time increments. Equations pertinent to time increments 1 through 62 are located in range D18 to IP67. Equations pertinent to time increments 63 through 124 are located in range G107 to IT156.

The first time increment (range D18 to F67) contains, for each of the 50 depth increments, an aqueous and sorbate contaminant concentration based on the dry weight concentrations in soil and apparent partition coefficient supplied by the user. The equations from which these concentrations are estimated are:

$$C_{aq} = \frac{(B)(C_{soil})}{(B)(K_{app}) + (P_w)} \quad [1]$$

$$C_{sorb} = (K_{app})(C_{aq}) \quad [2]$$

where; C_{soil} = total contaminant concentration in soil (mg/kg dry weight)

C_{aq} = aqueous concentration of contaminant in mg/l

C_{sorb} = sorbate concentration of contaminant in mg/kg
(more properly the concentration that is non-aqueous)

K_{app} = apparent partition coefficient in ml/g
(mathematically the ratio of C_{sorb} to C_{aq})

P_w = water-filled porosity of soil

B = dry bulk density of soil in g/cc

The second and all subsequent time increments contain for each of the 50 depth increments four different estimated values. These include a total contaminant concentration in soil, the total aqueous concentration, and the sorbate concentration.

The soil concentration in the first depth increment is estimated by subtracting the mass lost from soil in the previous time increment by solubilization into infiltrating water (the mass lost having migrated to the second depth increment). The aqueous concentration in the first depth increment is estimated with the use of equation [1] above. The sorbate concentration in the first depth increment is estimated with the use of equation [2] above.

The contaminant concentrations and other values estimated in the subsequent depth increments are based simply on balancing the mass of contaminant as it solubilizes from soil in one depth increment into infiltrating water and migrates vertically into the next depth increment. The original mass of contaminant remains constant, but the location of the contaminant changes with time.

The value of the time increment in cell B12 is simply the amount of time for infiltrating water to pass through the given depth increment based on the recharge rate and water-filled porosity of the soil.

Spreadsheet output: The most significant output includes cell B12 and the range C203 to DV252. Cell B12 is the time increment value in months which is estimated from the input values for the depth increment, recharge rate, and water-filled porosity of soil.

Range C203 to DV252 contains the estimated pore water contaminant concentrations at various depths at various times. Column C is for the first time increment. Column D is for the second time increment and so on. Column DV is for the 124th (and last) time increment. In order to assign a time value for each of these increments, it is necessary to multiply by the value entered in cell B12.

Similarly, row 203 (beginning at column C) pertains to soil pore water in the first depth increment. Row 204 (beginning at column C) pertains to the second depth increment and so on. Row 252 pertains to the 50th (and last) depth increment. In order to assign a depth value to each of these increments, it is necessary to multiply by the value entered in cell B10.

As already discussed, the calculations and additional estimates upon the values in range C203 to DV252 are based are included in the range D18 to IT156. They have been placed in range C203 to DV252 so that the migration trend of the contaminant through time can be easily discerned and so that the trend can be displayed graphically.

Example 1: A soil with the following properties is contaminated with lead at a dry weight concentration of 5000 mg/kg.

Bulk density = 1.5 g/cc
Water-filled porosity = 0.25

Recharge rate = 33 cm/yr [13 inches/yr]
Depth increment = 1 foot

The apparent partition coefficient is 50 (calculated from on-site soil data), and the approximated method detection limit for lead is 0.001mg/l.

The results of these inputs show that after 124 time increments (343 months or approximately 29 years) the greatest depth that lead has migrated beyond the initially contaminated one foot depth increment at a detectable level is about five feet. Approximately 66% of the lead remains in the initially contaminated one foot depth increment with 33% existing in the two feet below this increment.

Example 2: Suppose this scenario is the same as that of Scenario 1 except that the initial lead concentration in soil is 600 mg/kg.

The results of these inputs show that after 124 time increments (343 months or approximately 29 years) the greatest depth that lead has migrated beyond the initially contaminated one foot depth increment at a detectable level in soil pore water is about four feet. Again, approximately 66% of the lead remains in the initially contaminated one foot depth increment with 33% existing in the two feet below this increment.